The exact probability distribution of saturating states in random sequential adsorption

Masatomo Iwasa and Kyohei Fukuda

Department of Physics, Nagoya University

Nagoya, 464-8602, Japan

(Dated: December 3, 2008)

We consider the non-overlapping irreversible random sequential adsorption (RSA) process on one-dimensional finite line, which is known also as the car parking process. The probability of each coverage in saturating states is analytically and exactly obtained. In the derivation, a new representation of states in RSA process is introduced, which effectively works to make the calculation clear and simple.

PACS numbers: 02.50.-r, 68.43.De, 05.20.-y, 81.10.Aj

I. INTRODUCTION

We often see in various scientific and sociological fields that identical objects are sequentially placed at random on a region [1] . Then, a meaningful question naturally arise: How much of the region is finally covered by them? That kind of phenomenon is known as a non-overlapping irreversible random sequential adsorption (RSA), and the theories have been mainly developed in the field (see [1] and references therein). It has been found that in arbitrary dimension, RSA process reach a saturating or jamming configuration, where further adsorption events are not possible. The final coverage as well as the temporal approach to the saturating state are of interest [1, 2, 3, 4, 5, 6, 7, 8]. Exact analytical results have been obtained mainly in one dimension, where the problem is also known as the parking problem [1, 2, 3, 4].

In those previous works, while the mean coverage has been obtained, the probability for each coverage in saturating states has never been revealed. Deriving it on one-dimensional RSA process analytically and exactly is the main purpose of this paper.

II. THE MAIN RESULT

Suppose identical particles of unit length are placed sequentially at random on an interval of length l, subject to the constraint of no overlap. Here "place particles at random" means in this paper that each of them is placed based on the uniform distribution only on those empty spaces that have enough length to be placed. Note that it is not necessary to take the probability of finding already occupied place into account because we are not interested in the kinetics but only in the saturating states here. Then, the primary aim of this study is to obtain the probability of saturating states where there are n particles. The following is the main result, and its derivation is accomplished through this paper.

In RSA process as above, the probability of saturating states where there are n particles on the interval of length l becomes

$$P_{l,n} = \left[\prod_{r=0}^{n-1} (1 - Q_{l,r}) \right] Q_{l,n}, \ (0 < n \le l). \qquad (1)$$

Here

$$Q_{l,r} := \begin{cases} 0, & r \le \frac{l-1}{2}, \\ \sum_{k=0}^{\lfloor l-r \rfloor} (-1)^k {}_{r+1}C_k \left(1 - \frac{k}{l-r}\right)^r, & \frac{l-1}{2} < r \le l, \end{cases} \qquad (2)$$

where ${}_nC_r := \frac{n!}{r!(n-r)!}$ *and* $\lfloor \cdots \rfloor$ *denotes the floor function.*

III. THE PROOF

Let us introduce some notations which are used throughout this paper. Suppose now there are n particles on the interval of length l. Then the state can be represented by a point in $\mathbb{R}^{n+1}$. Namely, if we arrange the each length of $n + 1$ empty spaces between particles and between particles at the ends and the edges of the interval from the left side to the other, all of the states can be represented by a set of $n+1$ positive real number, say

$$(a_0, a_1, \ldots, a_n); \ 0 \le a_i, \ i = 0, 1, \ldots, n. \qquad (3)$$

An example of this notation is shown in Fig. 1.

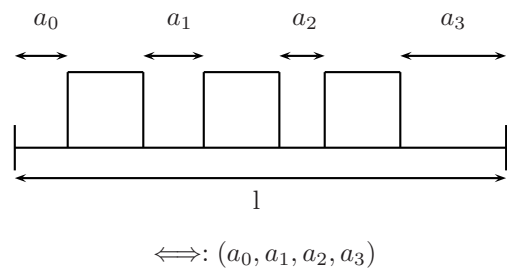$$\Longleftrightarrow: (a_0, a_1, a_2, a_3)$$

Fig. 1. The representation of states: The state illustrated above where $n = 3$ is expressed as $(a_0, a_1, a_2, a_3) \in \mathbb{R}^4$.

Because the length of the interval is l, a_i ($i = 0, 1, \ldots, n$) satisfies

$$\sum_{j=0}^{n} a_j = l - n. \tag{4}$$

Thanks to the constraint condition (4), the number of independent valuables is reduced. Henceforth in this paper we eliminate a_0. Thus, any state where there are n particles can be represented by a point in $S_{n,l-n}$,

$$(a_1, \ldots, a_n). \tag{5}$$

Here $S_{n,p} \subset \mathbb{R}^n$ ($0 < p$) is defined as

$$S_{n,p} := \left\{ (a_1, \ldots, a_n) \,\middle|\, \begin{array}{l} 0 \leq a_i, \quad (i = 1, \ldots, n), \\ \sum_{j=1}^{n} a_j \leq p \end{array} \right\}. \tag{6}$$

In $S_{n,l-n}$, let us find the subset where all points correspond to saturating states. Those are such states that any length of $n + 1$ empty spaces are less than 1. Therefore, the subset corresponds to $R_{n,l-n}$. Here $R_{n,p} \subset \mathbb{R}^n$ ($0 < p$) is defined as

$$R_{n,p} := \left\{ (a_1, \ldots, a_n) \,\middle|\, \begin{array}{l} 0 \leq a_i < 1, \ (i = 1, \ldots, n) \\ p - 1 < \sum_{j=1}^{n} a_j \leq p \end{array} \right\}. \tag{7}$$

On the other hand, all points in $S_{n,l-n} \backslash R_{n,l-n}$ satisfy $1 \leq a_i$ for some $i = 0, 1, \ldots, n$. That is to say, states corresponding to them are not saturating states, and another particle can be placed on the interval.

Next we discuss the probability of saturating states where there are n particles on the interval of length l. The derivation of the main result consists of three lemmas. At first, we see the following lemma.

Lemma 1. *Suppose the particles are placed at random on the interval. Then, in terms of the notation (5), each state represented by a point in $S_{n,l-n}$ has the same the probability.*

Proof. The proof is accomplished by mathematical induction. When $n = 1$, the event is placing a particle on the interval which is vacant. Therefore, the claim is obviously true by means of the definition of "at random", which is definitely described before the statement of the main result. Assume the lemma is true when $n = k$ for $k = 1, 2 \ldots$. Then we can show the lemma is also true when $n = k + 1$ as below. Any state represented by a point in $S_{k+1,l-(k+1)}$, say $(a_1, \ldots, a_{k+1})$ according to the notation (5), occurs if and only if a particle is placed in one of the $k + 1$ different states represented by $(a_2, a_3, \ldots, a_{k+1})$, $(a_1 + a_2 + 1, a_3, \ldots, a_{k+1})$, $(a_1, a_2 + a_3 + 1, \ldots, a_{k+1})$, $\cdots$, $(a_1, a_2, \ldots, a_k + a_{k+1} + 1)$, all of which are points in $S_{k,l-k}$. For example, a state $(3/2, 2/5, 5/4)$ occurs if and only if a particle is placed in one of $(2/5, 5/4)$, $(19/10, 5/4)$ or $(3/2, 33/20)$. In short, any point in $S_{k+1,l-(k+1)}$ is mapped from $k + 1$ different points in $S_{k,l-k}$ by placing a particle. From the assumption of the lemma, these $k + 1$ mapping have the same probability. Therefore, it has been proved that each state

represented by a point in $S_{k+1,l-(k+1)}$ has the same probability if so does each state in $S_{k,l-k}$. Thus, it has been inductively proved the lemma holds for all n. □

Now we can calculate the probability of saturating states where there are n particles. In what follows, $V(A)$ denotes the volume of domain A. Suppose there are n particles on the interval. Then, from Lemma 1, the conditional probability that this state is a saturating state in this given situation becomes

$$\frac{V(R_{n,l-n})}{V(S_{n,l-n})}. \tag{8}$$

On the other hand, the conditional probability that another particle can be added to this state becomes

$$\frac{V(S_{n,l-n} \backslash R_{n,l-n})}{V(S_{n,l-n})}. \tag{9}$$

Therefore, the probability of saturating states where there are n particles on the interval of length l, $P_{l,n}$, becomes,

$$\begin{aligned} P_{l,n} &= \left[\prod_{r=0}^{n-1} \frac{V(S_{r,l-r} \backslash R_{r,l-r})}{V(S_{r,l-r})} \right] \frac{V(R_{n,l-n})}{V(S_{n,l-n})}, \\ &= \left[\prod_{r=0}^{n-1} \left(1 - \frac{V(R_{r,l-r})}{V(S_{r,l-r})} \right) \right] \frac{V(R_{n,l-n})}{V(S_{n,l-n})}. \end{aligned} \tag{10}$$

What should be done to complete the derivation of the main result is to prove $\frac{V(R_{n,l-r})}{V(S_{n,l-r})}$ is equal to $Q_{l,r}$ in Eq. (2). Then, let us calculate $V(S_{n,p})$ and $V(R_{n,p})$. These are shown in Lemma 2 and Lemma 3.

Lemma 2.

$$V(S_{n,p}) = \frac{p^n}{n!}. \tag{11}$$

Proof. The domain $S_{n,p}$ reads

$$S_{n,p} = \left\{ (a_1, \ldots, a_n) \,\middle|\, \begin{array}{l} 0 \leq a_i \leq p - (a_1 + \cdots + a_{i-1}), \\ (i = 2, \ldots, n), \\ 0 \leq a_1 \leq p \end{array} \right\} \tag{12}$$

Therefore, the volume of $S_{l,p}$ becomes

$$\begin{aligned} V(S_{n,p}) &= \int_0^p da_1 \int_0^{p-a_1} da_2 \cdots \int_0^{p-(a_1+\cdots+a_{n-1})} da_n, \\ &= \frac{p^n}{n!}. \ \square \end{aligned} \tag{13}$$

By virtue of Lemma 2, let us find the volume of $R_{n,p}$.

Lemma 3.

$$V(R_{n,p}) = \begin{cases} 0, & (n \leq p - 1), \\ \sum_{k=0}^{\lfloor p \rfloor} (-1)^k {}_{n+1}C_k \frac{(p-k)^n}{n!}, & (p - 1 < n). \end{cases} \tag{14}$$

Proof. First of all, let us obtain the volume of

$$T_{n,p} := \left\{ (a_1, \ldots, a_n) \,\middle|\, \begin{array}{l} 0 \leq a_i < 1 \ (i = 1, \ldots, n) \\ \sum_{j=1}^{n} a_j \leq p \end{array} \right\}. \tag{15}$$

Once we obtain $V(T_{n,p})$, $V(R_{n,p})$ is calculated from $V(R_{n,p}) = V(T_{n,p}) - V(T_{n,p-1})$. To obtain the volume of $T_{n,p}$, we subtract the superfluous domain from $S_{n,p}$. In this way, it follows

$$
\begin{aligned}
V(T_{n,p}) = {} & V(S_{n,p}) - \sum_{1 \leq i_1 \leq n} V(U_{n,p}^{i_1}) + \sum_{1 \leq i_1 < i_2 \leq n} V(U_{n,p}^{i_1 i_2}) \\
& + \cdots + (-1)^k \sum_{1 \leq i_1 < \ldots < i_k \leq n} V(U_{n,p}^{i_1 \ldots i_k}) \\
& + \cdots + (-1)^{\lfloor p \rfloor} \sum_{1 \leq i_1 < \ldots < i_{\lfloor p \rfloor} \leq n} V(U_{n,p}^{i_1 \ldots i_{\lfloor p \rfloor}}).
\end{aligned}
\tag{16}
$$

Here we have introduced for $k = 1, \ldots, \lfloor p \rfloor$,

$$
U_{n,p}^{i_1 i_2 \ldots i_k} := \left\{ (a_1, \ldots, a_n) \ \middle| \ \begin{array}{l} 1 \leq a_i (i = i_1, \ldots, i_k), \\ 0 \leq a_i (i \neq i_1, \ldots, i_k), \\ \sum_{j=1}^{n} a_j \leq p \end{array} \right\}, \tag{17}
$$

Note that the formula (16) is suitable only for $\lfloor p \rfloor \leq n$, that is $p \leq n+1$. This is understandable if we concretely consider for n=3 as a simple example. For $n + 1 < p$, from the definition of $T_{n,p}$ (15), it obviously follows

$$
V(T_{n,p}) = 1. \tag{18}
$$

Let us calculate the right hand side of Eq. (16). For any combination of $(i_1, \ldots, i_k)$,

$$
V(U_{n,p}^{i_1 i_2 \ldots i_k}) = V(U_{n,p}^{12 \ldots k}), \tag{19}
$$

because of the symmetry with respect to the permutation of upper indices. Then, it follows

$$
\sum_{1 \leq i_1 < \ldots < i_k \leq n} V(U_{n,p}^{i_1 i_2 \ldots i_k}) = {}_n C_k V(U_{n,p}^{12 \ldots k}). \tag{20}
$$

Therefore, Eq. (16) reads

$$
V(T_{n,p}) = V(S_{n,p}) + \left(\sum_{k=1}^{\lfloor p \rfloor} (-1)^k {}_n C_k V(U_{n,p}^{12 \ldots k}) \right) \tag{21}
$$

Let us obtain the volume of $U_{n,p}^{1 \ldots k}$. With the transformation

$$
\tilde{a}_i := \left\{ \begin{array}{ll} a_i - 1, & (i = 1, \ldots, k), \\ a_i, & (i = k+1, \ldots, n), \end{array} \right. \tag{22}
$$

$U_{n,p}^{1, \ldots, k}$ is written by

$$
\left\{ (\tilde{a}_1, \ldots, \tilde{a}_n) \ \middle| \ \begin{array}{l} 0 \leq \tilde{a}_i (i = i_1, \ldots, n) \\ \sum_{j=1}^{n} \tilde{a}_j \leq p - k \end{array} \right\}, \tag{23}
$$

which corresponds to $S_{n,p-k}$. Therefore, since the Jacobian of the transformation is one, we obtain with the aid of Lemma 2

$$
V(U_{n,p}^{1 \ldots k}) = V(S_{n,p-k}), \tag{24}
$$

$$
= \frac{(p-k)^n}{n!}. \tag{25}
$$

By substituting Eq. (13) and Eq. (25) into Eq. (21), and according to Eq. (18), we obtain

$$
V(T_{n,p}) = \left\{ \begin{array}{ll} 1, & (n \leq p - 1), \\ \sum_{k=0}^{\lfloor p \rfloor} (-1)^k {}_n C_k \frac{(p-k)^n}{n!}, & (p - 1 < n). \end{array} \right. \tag{26}
$$

Hence, we can immediately show that Eq. (14) holds according to $V(R_{n,p}) = V(T_{n,p}) - V(T_{n,p-1})$, noting that $V(T_{n,p}) = 1$ for $\lfloor p \rfloor = n$ while Eq. (16) holds. $\square$

As noted before, what must be done to complete the derivation of the main result is to show that $\frac{V(R_{r,l-r})}{V(S_{r,l-r})}$ is equal to $Q_{l,r}$ in Eq. (2). By substituting Eq. (11) and Eq. (14), We can immediately show that

$$
\frac{V(R_{n,p})}{V(S_{n,p})} = \left\{ \begin{array}{ll} 0, & (n \leq p - 1), \\ \sum_{k=0}^{\lfloor p \rfloor} (-1)^k {}_{n+1} C_k \left(1 - \frac{k}{p} \right)^n, & (p - 1 < n). \end{array} \right. \tag{27}
$$

IV. CONCLUDING REMARKS

The RSA model on one-dimensional finite interval has been analyzed exactly. As a result, the probability of each coverage at saturating states has been obtained explicitly for a generic system. Then we can obtain the explicit expression of all moments. The main result, that is exact probability for any system size, would be useful for explaining the various actual RSA phenomena since experiments are always carried out on a system of finite size. Compared with the previous studies [1, 2, 3, 4, 5, 6, 7, 8], this study takes another way to represent a state during the adsorbing process. Through the derivation of the main result, we see that this notation effectively works to make the calculation clear and simple. Besides this, omitting the kinetics also seems to be an important point to obtain the result. However, since we are almost always interested in not only final states but also kinetics in physics, construction of an appropriate master equation utilizing this result seems to be an significant problem for the future. The consistency with the previous studies [1, 2, 3, 4, 5, 6, 7, 8] is another question. This should be investigated, if possible, by obtaining the asymptotic behavior of the mean coverage, that is the average of n/l, for $l \to \infty$.

[1] For comprehensive review see J. W. Evans, *Rev. Mod. Phys.* **65** 1281, (1993)

[2] A. Rényi, *Publ. Math. Inst. Hung. Acad. Sci* **3** 109, (1958)

[3] B. Widom, *J. Chem. Phys* **44** 3888, (1966)

[4] J. J. Gonzalez, P. C. Hemmer and J. S. hoye, *Chem. Phys.* **3** 228, (1974)

[5] J. Feder, *J. Theor. Biol.* **87** 237, (1980)

[6] Y. Pomeau, *J. Phys. A* **13** L193, (1980)

[7] R. H. Swendsen, *Phys. Rev. A* **24** 504, (1981)

[8] E. L. Hinrichsen, J. Feder and T. Jossang, *J. stat. phys.* **44** 793, (1986)